COMPUTER METHODS FOR SOLVING A DIFFUSION BOUNDARY VALUE PROBLEM

by
V. S. GYLYS

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Electrical Engineering Research Laboratory
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University of Illinois
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1. INTRODUCTION

This report describes three finite difference methods and a computer program for a boundary value problem which models the density of electrons in the ionosphere. Let the variables H and T represent the altitude (height) and time, respectively; let N = N(H,T) represent the electron density in the ionosphere. Then this boundary value problem can be expressed in terms of the parabolic differential equation

$$\frac{\partial N}{\partial t} = a(H,T)\frac{\partial^2 N}{\partial u^2} + b(H,T)\frac{\partial N}{\partial H} + [c(H,T) + d(H,T,N)] \cdot N + q(H,T) , \qquad (1.1)$$

where $0 \le H \le H^*$ and T > 0, together with the following boundary conditions:

(a)
$$N(0,T) = 0$$
 for $T > 0$; (1.1a)

(b)
$$\frac{\partial N}{\partial H} + kN = 0$$
 at $H = H^*$ for $T > 0$; (1.1b)

(c)
$$N(H,0) = g_i(H)$$
 for $0 \le H = H^*$, where g_i is a known function of H and $i = 1$ or 2 . (1.1c)

For the special case to be considered in this report, the differential equation (1.1) can be simplified to

$$\frac{\partial N}{\partial T} = a(H)\frac{\partial^2 N}{\partial H^2} + b(H)\frac{\partial N}{\partial H} + e(H) \cdot N + q(H, T)$$
 (1.2)

We shall be interested in numerical solutions of this boundary value problem for the values of T restricted to $0 < T \le T^*$, where T^* is some time constant (typically, $T^* = 24$ hours).

Next we shall briefly outline the contents of this report. Section 2

discusses a normalization of the independent variables, H and T, and then formally restates the boundary value problem (1.1a) - (1.2) in terms of the transformed variables. Section 3 begins with an explanation of the notation and other concepts used in the formulation of the finite difference equations; then it briefly mentions some theoretical aspects, such as convergence, of the three finite difference methods to be introduced in Sections 4, 5, and 6. Appendices A, B, C, and D describe and illustrate the IBM 7094 computer program. Appendix A gives the expressions needed for the computation of the coefficients of the differential equation and of the boundary conditions.

2. NORMALIZATION OF INDEPENDENT VARIABLES

For positive constants H* and T*, set

$$h = \frac{H}{H^*} \quad \text{and} \quad t = \frac{T}{T^*} \quad . \tag{2.1}$$

Since $0 \le H \le H^*$ and T > 0, we have $0 \le h \le 1$ and $0 < t \le 1$ if $T \le T^*$). The partial derivatives in the equation (1.1) or (1.2) can now be expressed in terms of the normalized independent variables, h and t, as follows:

$$\frac{\partial N}{\partial H} = \frac{\partial N}{\partial h} \cdot \frac{dh}{dH} = \frac{\partial N}{\partial h} \cdot \frac{1}{H^*} , \qquad (2.2)$$

$$\frac{\partial^2 N}{\partial H^2} = \frac{\partial}{\partial H} \left[\frac{\partial N}{\partial H} \right] = \frac{\partial}{\partial h} \left[\frac{\partial N}{\partial h} \cdot \frac{1}{H^*} \right] \cdot \frac{dh}{dH} = \frac{\partial^2 N}{\partial h^2} \cdot \frac{1}{(H^*)^2} , \qquad (2.3)$$

and

$$\frac{\partial N}{\partial T} = \frac{\partial N}{\partial t} \cdot \frac{dt}{dT} = \frac{\partial N}{\partial t} \cdot \frac{1}{T*} \qquad (2.4)$$

Consequently, the boundary value problem will now formally be written in the form

$$\frac{\partial N}{\partial t} = A(h) \frac{\partial^2 N}{\partial h^2} + B(h) \frac{\partial N}{\partial h} + E(h) N + Q(h, t) , \qquad (2.5)$$

where $0 \le h \le 1$ and t > 0, with the boundary conditions:

(a)
$$N(0,t) = 0$$
; (2.5a)

(b)
$$\frac{\partial N}{\partial h} + \frac{1}{2H_1} \cdot N = 0$$
 at $h = 1$ for $t > 0$; (2.5b)

(c)
$$N(h,0) = G_i(h)$$
 for $0 \le h \le 1$, where G_i is a given function (2.5c) of h and $i = 1$ or 2.

From now on when referring to the boundary value problem we shall have in mind the system described by the equations (2.5) through (2.5c). Expressions for computing the coefficients that appear in this system are given in APPENDIX A. The same appendix also contains information on the dimensional units used.

3. FINITE DIFFERENCE METHODS

Consider the normalized independent variables h and t. Let L be a positive integer (to be provided as an input parameter). Introduce a rectangular grid over the region R,

$$t \geq 0$$
 and $0 \leq h \leq 1$, (3.1)

in the ht-plane by subdividing R into rectangles of sides

$$\triangle h = \frac{1}{L}$$
 and $\triangle t$.

Here the time step $\triangle t$ is a positive real number and an input quantity. Then the coordinates (h,t) of a representative grid point P are

$$h = i \cdot \Delta h$$
, $i = 0, 1, 2, ..., L$ (3.2)

and

$$t = n \cdot \Delta t$$
, $n = 0, 1, 2, ...$ (3.3)

The coordinates of $P_{i,n}$ often will be written (h_i, t_n) .

In general, we shall use the subscripts (i,n) for referring to the value at $P_{i,n}$ of any quantity which is a function of h and t. Thus we shall write $N_{i,n}$ for $N(h_i, t_n)$, the value at $P_{i,n}$ of the exact (analytic) solution of our boundary value problem. To cite another example, A_i will denote the value at $P_{i,n}$ of the coefficient A(h) of the partial differential equation; in the present case, the second subscript, n, is missing because A is independent of t.

Let the numbers W represent the exact solution of any one of the three finite difference schemes (backward difference, central difference, or Crank-Nicolson method). Here we use the adjective "exact" because as is well known

a numerical solution obtained on a digital computer will normally contain round-off error and thus will differ from the numbers $W_{i,n}$.

The finite difference equations for the three approximation methods used by us are derived in the ensuing sections of this report. At this point one should note only the following.

1. Each of the three finite difference methods leads to a system

$$\widetilde{MW}_{n+1} = \overline{U}(\widetilde{W}_n) \tag{3.4}$$

of linear equations, where M is a tridiagonal matrix. In the equation (3.4), \overline{W}_n represents the column vector consisting of the numbers $W_{i,n}$ ($i=1,2,\ldots,L$). Our computer program solves this system of equations by using a well known version of Guassian elimination method specially adapted to tridiagonal matrices (see, for example, the reference [2], p. 104). If further investigation of the computational results indicated a need of different techniques to solve the resulting system of linear equations, our computer program has been so designed that any such method (an iterative technique, for example) could easily replace the present Gaussian elimination procedure. We may also mention here that the program uses double precision floating point arithmetic. On the IBM 7094, this gives floating point numbers with the mantissas 54 bits long.

2. No theoretical treatment of the stability, compatability (also called consistency by some authors), and convergence properties of the finite difference schemes used by us has been included in this report. These problems are presently under investigation and will be summarized in a forth-coming paper. For the time being the reader may refer to any of the four

references listed at the end of this report: they treat these theoretical questions for similar (but not exactly our) boundary value problems.

4. THE BACKWARD DIFFERENCE METHOD

The backward (implicit) difference analog of (2.5) is

$$\frac{\mathbf{w}_{i,n+1} - \mathbf{w}_{i,n}}{\triangle t} = \mathbf{A}_{i} \left[\frac{\mathbf{w}_{i+1,n+1} - 2\mathbf{w}_{i,n+1} + \mathbf{w}_{i-1,n+1}}{(\triangle h)^{2}} \right] + \mathbf{B}_{i} \left[\frac{\mathbf{w}_{i+1,n+1} - \mathbf{w}_{i-1,n+1}}{2(\triangle h)} \right] + \mathbf{E}_{i} \mathbf{w}_{i,n+1} + \mathbf{Q}_{i,n+1} .$$
(4.1)

Write $r = \triangle t/(\triangle h)^2$. Then

$$-[(\triangle t)Q_{i,n+1} + W_{i,n}] = r[A_i - \frac{\triangle h}{2} B_i] W_{i-1,n+1} +$$

$$+ [-2rA_i + (\triangle t) E_i - 1] W_{i,n+1} + r[A_i + \frac{\triangle h}{2} B_i] W_{i+1,n+1} .$$

$$(4.2)$$

Thus for $n \ge 0$ and for $i = 1, 2, \dots, L-1$ we can write

$$P_{i} W_{i-1,n+1} + R_{i} W_{i,n+1} + S_{i} W_{i+1,n+1} = U_{i,n+1},$$
 (4.3)

where due to the boundary conditions at h = 0 we can set

$$P_1 = 0$$
; (4.4a)

the other coefficients for $i \leq L - 1$ can be written by comparing (4.2) with (4.3):

$$P_i = r[A_i - \frac{\Delta h}{2} B_i]$$
 for $i = 2, 3, ..., L-1$; (4.4b)

$$R_{i} = [-2r A_{i} + (\triangle t) E_{i} - 1]$$
 for $i = 1, 2, ..., L-1$; (4.4c)

(4.7)

$$S_i = r[A_i + \frac{\Delta h}{2} B_i]$$
 for $i = 1, 2, ..., L-1$; (4.4d)

and

$$U_{i,n+1} = -[(\triangle t) Q_{i,n+1} + W_{i,n}]$$
 for $i = 1, 2, ..., L-1$. (4.4e)

Obtain the coefficients of the equation

$$P_{L} W_{L-1, n+1} + R_{L} W_{L, n+1} = U_{L, n+1}$$
 (4.5)

from the boundary condition

$$\frac{\partial N}{\partial h} + \frac{1}{2H_1} N = 0$$

at h=1. The central difference representation with an accuracy of $0(h^2)$ of this boundary condition at t_{n+1} is

$$\frac{W_{L+1,n+1} - W_{L-1,n+1}}{2(\triangle h)} + \frac{1}{2H_1} W_{L,n+1} = 0$$

or

$$W_{L+1,n+1} = -\frac{(\triangle h)}{H_1} W_{L,n+1} + W_{L-1,n+1}$$
 (4.6)

On the other hand, the backward difference equation (4.2) for i = L is

$$-[(\triangle t) Q_{L, n+1} + W_{L, n}] = r[A_{L} - \frac{\triangle h}{2} B_{L}] W_{L-1, n+1} +$$

$$+[-2rA_{L} + (\triangle t) E_{L} - 1] W_{L, n+1} + r[A_{L} + \frac{\triangle h}{2} B_{L}] W_{L+1, n+1} .$$

Replacing $W_{L+1,n+1}$ in (4.7) by the right-hand side of (4.6) we get

-[(
$$\triangle t$$
) $Q_{L,n+1} + W_{L,n}$] = $r[A_L - \frac{\triangle_h}{2} B_L] W_{L-1,n+1} +$

$$+[-2rA_{L} + (\triangle t) E_{L} - 1] W_{L,n+1} + r[A_{L} + \frac{\triangle h}{2} B_{L}] \cdot [-\frac{\triangle h}{H_{1}} W_{L,n+1} + W_{L-1,n+1}].$$

Hence

$$P_{L} W_{L-1, n+1} + R_{L} W_{L, n+1} = U_{L, n+1}$$
, (4.8)

where:

$$P_{L} = 2rA_{L} ; \qquad (4.9a)$$

$$R_{L} = -2rA_{L} + (\triangle t)E_{L} - 1 - \frac{r(\triangle h)}{H_{1}}A_{L} - \frac{r(\triangle h)^{2}}{2H_{1}}B_{L}$$

$$= -rA_{L}[2 + \frac{\triangle h}{H_{1}}] + (\triangle t)[E_{L} - \frac{1}{2H_{1}}B_{L}] - 1; \qquad (4.9b)$$

$$U_{L, n+1} = -[(\triangle t) Q_{L, n+1} + W_{L, n}]$$
 (4.9c)

5. A CENTRAL DIFFERENCE METHOD BASED ON THREE TIME LEVELS

Since the coefficients A, B, and E of the differential equation (2.5) are independent of t and N, a central difference representation of (2.5) can be written in the form

$$\triangle_{t} W_{i,n} = \frac{A_{i}}{3} \cdot \triangle_{h}^{2}(W_{i,n+1} + W_{i,n} + W_{i,n-1}) +$$

$$+\frac{B_{i}}{3} \cdot \triangle_{h}(W_{i,n+1} + W_{i,n} + W_{i,n-1}) + E_{i} \cdot W_{i,n} + Q_{i,n}$$
 (5.1)

Here

$$\triangle_{h}^{2}W_{i,j} = \frac{W_{i+1,j} - 2W_{i,j} + W_{i-1,j}}{(\triangle h)^{2}}, \qquad (5.1a)$$

$$\triangle_{h}W_{i,j} = \frac{W_{i+1,j} - W_{i-1,j}}{2(\triangle h)} , \qquad (5.1b)$$

and

$$\triangle_{t}W_{i,j} = \frac{W_{i,j+1} - W_{i,j-1}}{2(\triangle t)}$$
 (5.1c)

are the finite difference approximations to $\frac{\partial^2 w}{\partial h^2}$, $\frac{\partial w}{\partial h}$, and $\frac{\partial w}{\partial t}$, respectively, at $(h,t)=(h_i,t_j)$. By expanding (5.1) in terms of these approximations and by, as before, writing $r=\frac{(\triangle t)}{(\triangle h)^2}$, we get

$$3(W_{i,n+1} - W_{i,n-1}) = 2A_{i}r[(W_{i+1,n+1} - 2W_{i,n+1} + W_{i-1,n+1}) +$$

+
$$(W_{i+1,n} - 2W_{i,n} + W_{i-1,n}) + (W_{i+1,n-1} - 2W_{i,n-1} + W_{i-1,n-1})]$$
 +

$$+ B_{i} \frac{\triangle t}{\triangle h} [(W_{i+1,n+1} - W_{i-1,n+1}) + (W_{i+1,n} - W_{i-1,n}) +$$

+
$$(W_{i+1,n-1} - W_{i-1,n-1})] + 6(\Delta t)[E_iW_{i,n} + Q_{i,n}]$$

or

$$r[2A_{i} - (\triangle h)B_{i}] W_{i-1,n+1} + [-4rA_{i} - 3] W_{i,n+1} +$$

$$+ r[2A_{i} + (\triangle h)B_{i}] W_{i+1,n+1} = -(2A_{i}r)[(W_{i+1,n} + W_{i+1,n-1}) -$$

$$-2(W_{i,n} + W_{i,n-1}) + (W_{i-1,n} + W_{i-1,n-1})] -$$

-
$$(B_i \frac{\Delta t}{\Delta h})[(W_{i+1,n} + W_{i+1,n-1}) - (W_{i-1,n} + W_{i-1,n-1})]$$
 -

$$- [6(\Delta t)(E_{i} W_{i,n} + Q_{i,n})] - 3 W_{i,n-1} . (5.2)$$

Thus we obtain L-1 equations

$$P_{i}W_{i-1,n+1} + R_{i}W_{i,n+1} + S_{i}W_{i+1,n+1} = U_{i,n+1}$$
(5.3)

for $n \ge 1$ and i = 1, 2, ..., L-1. Since $W_{0,j} = 0$, due to the boundary condition at h = 0, we can set

$$P_1 = 0 ; (5.4a)$$

the other coefficients for $i \leq L-1$ are:

$$P_{i} = r[2A_{i} - (\Delta h)B_{i}], \quad i = 2, 3, ..., L-1;$$
 (5.4b)

$$R_i = -[4rA_i + 3], \quad i = 1, 2, ..., L-1;$$
 (5.4c)

$$S_{i} = r[2A_{i} + (\triangle h)B_{i}], \quad i = 1, 2, ..., L-1;$$
 (5.4d)

and

$$\begin{split} \mathbf{U}_{i,n+1} &= -\mathbf{r} \bigg\{ \big[\, 2\mathbf{A}_{i} \, + \, (\triangle \mathbf{h}) \, \mathbf{B}_{i} \, \big] \, (\mathbf{W}_{i+1,n} \, + \, \mathbf{W}_{i+1,n-1}) \, + \\ &\quad + \, \big[\, 2\mathbf{A}_{i} \, + \, (\triangle \mathbf{h}) \, \mathbf{B}_{i} \, \big] \, (\mathbf{W}_{i-1,n} \, + \, \mathbf{W}_{i-1,n-1}) \, - \, 4\mathbf{A}_{i} \, (\mathbf{W}_{i,n} \, + \\ &\quad + \, \mathbf{W}_{i,n-1}) \bigg\} \, - \, 6 \, (\triangle \mathbf{t}) \, \big[\, \mathbf{E}_{i} \, \mathbf{W}_{i,n} \, + \, \mathbf{Q}_{i,n} \, \big] \, - \, 3\mathbf{W}_{i,n-1} \, , \end{split}$$
 (5.4e)

$$i = 1, 2, \ldots, L-1$$

Remark: to evaluate $U_{1,n+1}$, set $W_{0,n-1} = W_{0,n} = 0$.

In order to obtain the coefficients of the Lth equation,

$$P_{L} \cdot W_{L-1, n+1} + R_{L} \cdot W_{L, n+1} = U_{L, n+1},$$
 (5.5)

use the central difference representation

$$\frac{W_{L+1,j} - W_{L-1,j}}{2(\triangle h)} + \frac{1}{2H_1} W_{L,j} = 0$$

of the boundary condition at $h = h_{T} = 1$; from this difference equation we get

$$W_{L+1,j} = -\frac{\triangle h}{H_1} W_{L,j} + W_{L-1,j}$$
 (5.6)

Next let i = L in (5.2) and replace the $W_{L+1,n}$ by the right-hand side of (5.6) with j = n - 1, n or n + 1 as required. Thus,

$$\begin{split} \mathbf{r} [\ 2\mathbf{A_L} - \ (\triangle h) \mathbf{B_L}] \ \mathbf{W_{L-1,\,n+1}} \ + \ [\ -4\mathbf{r} \mathbf{A_L} - \ 3 \] \ \mathbf{W_{L,\,n+1}} \ + \\ + \ \mathbf{r} [\ 2\mathbf{A_L} + \ (\triangle h) \mathbf{B_L}] (- \ \frac{\triangle h}{\mathbf{H_1}} \ \mathbf{W_{L,\,n+1}} + \mathbf{W_{L-1,\,n+1}}) \ = \\ & = - \ \mathbf{r} \left\{ [\ 2\mathbf{A_L} + \ (\triangle h) \mathbf{B_L}] \cdot [- \ \frac{\triangle h}{\mathbf{H_1}} (\mathbf{W_{L,\,n}} + \mathbf{W_{L,\,n-1}}) \ + (\mathbf{W_{L-1,\,n}} + \mathbf{W_{L-1,\,n-1}}) \ + \\ + \ [\ 2\mathbf{A_L} - \ (\triangle h) \mathbf{B_L}] (\mathbf{W_{L-1,\,n}} + \mathbf{W_{L-1,\,n-1}}) \ - \ 4\mathbf{A_L} (\mathbf{W_{L,\,n}} + \mathbf{W_{L,\,n-1}}) \right\} \ - \\ & - \ 6 (\triangle t) [\mathbf{E_L} \mathbf{W_{L,\,n}} + \mathbf{Q_{L,\,n}}] \ - \ 3\mathbf{W_{L,\,n-1}} \ . \end{split}$$

It follows that

$$P_{T} = 4rA_{T} , \qquad (5.7a)$$

$$R_{L} = -\left[2rA_{L}\left(2 + \frac{\Delta h}{H_{1}}\right) + \frac{(\Delta t)B_{L}}{H_{1}} + 3\right] , \qquad (5.7b)$$

and that

$$U_{L,n+1} = -r \left\{ 4A_{L}(W_{L-1,n} + W_{L-1,n-1}) - \left[2A_{L}(2 + \frac{\Delta h}{H_{1}}) + \frac{(\Delta h)^{2}}{H_{1}} B_{L} \right] (W_{L,n} + W_{L,n-1}) \right\} - -6(\Delta t) \left[E_{L}W_{L,n} + Q_{L,n} \right] - 3W_{L,n-1} .$$
 (5.7c)

THE CRANK-NICOLSON METHOD

In the present case, the finite difference representation of the differential equation (2.5) is

$$\frac{W_{i,n+1} - W_{i,n}}{\triangle t} = \frac{A_{i}}{2} \cdot \triangle_{h}^{2}(W_{i,n+1} + W_{i,n}) + \frac{B_{i}}{2} \cdot \triangle_{h}(W_{i,n+1} + W_{i,n}) + \frac{E_{i}}{2}(W_{i,n+1} + W_{i,n}) + \frac{Q_{i,n+1} + Q_{i,n}}{2},$$
(6.1)

where the operators \triangle_h^2 and \triangle_h are defined by (5.1a) and (5.1b), respectively. Then writing $r=\frac{\triangle t}{\left(\triangle h\right)^2}$, we have

$$\begin{split} 2[W_{i,n+1} - W_{i,n}] &= A_{i}r[(W_{i+1,n+1} - 2W_{i,n+1} + W_{i-1,n+1}) + \\ &+ (W_{i+1,n} - 2W_{i,n} + W_{i-1,n})] + \frac{B_{i}}{2}(\frac{\triangle t}{\triangle h})[(W_{i+1,n+1} - W_{i-1,n+1}) + \\ &+ (W_{i+1,n} - W_{i-1,n})] + [E_{i}(W_{i,n+1} + W_{i,n}) + (Q_{i,n+1} + Q_{i,n})]\triangle t \end{split}$$

which leads to

$$2[W_{i,n+1} - W_{i,n}] = A_i r[(W_{i+1,n+1} + W_{i+1,n}) + (W_{i-1,n+1} + W_{i-1,n}) - (W_{i,n+1} + W_{i,n})] + \frac{B_i}{2} (\frac{\triangle t}{\triangle h})[(W_{i+1,n+1} + W_{i+1,n}) - (W_{i+1,n+1} + W_{i+1,n})] + \frac{B_i}{2} (\frac{\triangle t}{\triangle h})[(W_{i+1,n+1} + W_{i+1,n})] + (W_{i+1,n+1} + W_{i+1,n})] + (W_{i+1,n+1} + W_{i+1,n}) - (W_{i+1,n+1} + W_{i+1,n})] + (W_{i+1,n+1} + W_{i+1,n}) + + (W_{i+1,n+1} + W_{i+1,n+1} + W_{i+1,n+1}) + (W_{i+1,n+1} + W_{i+1,n+1} + W_{i+1,n+1} + W_{i+1,n+1}) + (W_{i+1,n+1} + W_{i+1,n+1} + W_{i+1,$$

$$- (W_{i-1,n+1} + W_{i-1,n})] + [E_i(W_{i,n+1} + W_{i,n}) + Q_{i,n+1} + Q_{i,n})] \Delta t .$$

Therefore,

$$[rA_{i} - \frac{B_{i}}{2}(\frac{\Delta t}{\Delta h})]W_{i-1,n+1} + [-(2 + 2rA_{i}) + \Delta tE_{i}]W_{i,n+1} +$$

$$+ [rA_{i} + \frac{B_{i}}{2}(\frac{\Delta t}{\Delta h})]W_{i+1,n+1} =$$

$$= -\left\{ [rA_{i} - \frac{B_{i}}{2}(\frac{\Delta t}{\Delta h})]W_{i-1,n} + [2 - 2rA_{i} + \Delta tE_{i}]W_{i,n} + [rA_{i} + \frac{B_{i}}{2}(\frac{\Delta t}{\Delta h})]W_{i+1,n} + [Q_{i,n+1} + Q_{i,n}]\Delta t \right\}.$$

$$(6.2)$$

Hence for $n \ge 0$ and i = 1, 2, ..., L-1 we obtain L-1 equations

$$P_{i}^{W}_{i-1,n+1} + R_{i}^{W}_{i,n+1} + S_{i}^{W}_{i+1,n+1} = U_{i,n+1} . \tag{6.3}$$

Due to the boundary condition at h=0, we have $W_{0,j}=0$ for all j. Thus we can set

$$P_1 = 0.$$
 (6.4a)

Then the other coefficients for $i \leq L-1$ are as follows:

$$P_{i} = r[A_{i} - (\frac{\triangle h}{2})B_{i}], \quad i = 2,3,...,L-1;$$
 (6.4b)

$$R_{i} = \triangle tE_{i} - 2(1 + A_{i}r), \quad i = 1, 2, ..., L-1;$$
 (6.4c)

$$S_{i} = r[A_{i} + (\frac{\Delta h}{2})B_{i}], \quad i = 1, 2, ..., L-1;$$
 (6.4d)

and

$$\begin{aligned} \mathbf{U}_{i,n+1} &= -\mathbf{r} [\mathbf{A}_{i} - (\frac{\triangle h}{2}) \mathbf{B}_{i}] \mathbf{W}_{i-1,n} + [\triangle t \mathbf{E}_{i} + 2(1 - \mathbf{r} \mathbf{A}_{i})] \mathbf{W}_{i,n} + \\ &+ \mathbf{r} [\mathbf{A}_{i} + (\frac{\triangle h}{2}) \mathbf{B}_{i}] \mathbf{W}_{i+1,n} + (\mathbf{Q}_{i,n+1} + \mathbf{Q}_{i,n}) \triangle t , \\ &+ \mathbf{I} &= 1, 2, \dots, L-1 . \end{aligned}$$
 (6.4e)

Remark: to evaluate $U_{1,n+1}$, use $W_{0,n} = 0$.

In order to obtain the coefficients of the L equation,

$$P_{L} \cdot W_{L-1, n+1} + R_{L} \cdot W_{L, n+1} = U_{L, n+1},$$
 (6.5)

use the central difference representation

$$\frac{W_{L+1, j} - W_{L-1, j}}{2(h)} + \frac{1}{2H_1} W_{L, j} = 0$$

of the boundary condition at $h = h_{I_i} = 1$; this difference equation implies

$$W_{L+1,j} = - \left(\frac{\triangle h}{H_1}\right) W_{L,j} + W_{L-1,j}$$
 (6.6)

Next set i=L in (6.2) and replace the $W_{L+1,\,j}$ by the right-hand side of (6.6), where j=n,n+1. This gives us

$$\begin{split} \left[\mathbf{r} \mathbf{A}_{L} - \frac{^{B}_{L}}{2} (\frac{\triangle t}{\triangle h}) \mathbf{W}_{L-1, n+1} \right] + \left[-2(1 + \mathbf{r} \mathbf{A}_{L}) + \triangle t \mathbf{E}_{L} \right] \mathbf{W}_{L, n+1} + \\ + \left[\mathbf{r} \mathbf{A}_{L} + \frac{^{B}_{L}}{2} (\frac{\triangle t}{\triangle h}) \right] \cdot \left[-(\frac{\triangle h}{H_{1}}) \mathbf{W}_{L, n+1} + \mathbf{W}_{L-1, n+1} \right] = \\ = -\left\{ \left[\mathbf{r} \mathbf{A}_{L} - \frac{^{B}_{L}}{2} (\frac{\triangle t}{\triangle h}) \right] \mathbf{W}_{L-1, n} + \left[2(1 - \mathbf{r} \mathbf{A}_{L}) + \triangle t \mathbf{E}_{L} \right] \mathbf{W}_{L, n} + \right. \\ + \left[\mathbf{r} \mathbf{A}_{L} + \frac{^{B}_{L}}{2} (\frac{\triangle t}{\triangle h}) \right] \cdot \left[-(\frac{\triangle h}{H_{1}}) \mathbf{W}_{L, n} + \mathbf{W}_{L-1, n} \right] + (\mathbf{Q}_{L, n+1} + \mathbf{Q}_{L, n}) \triangle t \right\} . \end{split}$$

It follows that

$$P_{L} = 2rA_{L}, \qquad (6.7a)$$

$$R_{L} = \left[-2 - 2rA_{L} + \triangle^{t}E_{L} - rA_{L}(\frac{\triangle h}{H_{1}}) - \frac{B_{L}}{2}(\frac{\triangle t}{\triangle h})(\frac{\triangle h}{H_{1}})\right]$$

$$= -\left[rA_{L}(2 + \frac{\triangle h}{H_{1}}) + \frac{B_{L}}{2}(\frac{\triangle t}{H_{1}}) + 2 - \triangle^{t}E_{L}\right], \qquad (6.7b)$$

and that

$$U_{L,n+1} = -\left\{ \left[2rA_{L}\right] W_{L-1,n} + \left[2 - 2rA_{L} + \triangle^{t}E_{L} - rA_{L}(\frac{\triangle^{h}}{H_{1}}) - \frac{B_{L}(\triangle^{t}}{\triangle^{h}}) (\frac{\triangle^{h}}{H_{1}}) \right] W_{L,n} + (Q_{L,n+1} + Q_{L,n}) \triangle^{t} \right\}$$

$$= -\left\{ \left[2rA_{L}\right] W_{L-1,n} + \left[-rA_{L}(2 + \frac{\triangle^{h}}{H_{1}}) - \frac{B_{L}}{2}(\frac{\triangle^{t}}{H_{1}}) + \frac{2 + \triangle^{t}E_{L}}{2} \right] W_{L,n} + (Q_{L,n+1} + Q_{L,n}) \triangle^{t} \right\}. \tag{6.7c}$$

7. REFERENCES

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APPENDIX A: COEFFICIENTS OF THE DIFFERENTIAL EQUATION AND OF THE BOUNDARY CONDITIONS IN TERMS OF THE INPUT PARAMETERS

A.1 The Input Parameters and their Dimensional Units

In order to specify the dimensions of the input parameters and the coefficients of the boundary value problem, let $\hat{\lambda}$ and $\hat{\tau}$ denote the units of height (length) and time, respectively. The normalized dimensional units for h and t used by the program internally are $1\hat{\lambda}=1,000$ kilometers and $1\hat{\tau}=24$ hours, respectively. The units of h and t to be used for external input are described in APPENDIX B.

The following parameters must be provided as a part of input information:

$$\begin{array}{lll} \mathbf{H}_0 & \text{in } [\widehat{\boldsymbol{\lambda}}] \ , \\ \mathbf{H}_1 & \text{in } [\widehat{\boldsymbol{\lambda}}] \ , \\ \mathbf{D}_0 & \text{in } [\widehat{\boldsymbol{\lambda}}^2/\widehat{\boldsymbol{\tau}}] \ , \\ \mathbf{Q}_0 & \text{in } [\widehat{\boldsymbol{\lambda}}^{-3} \cdot \widehat{\boldsymbol{\tau}}^{-1}] \ , \\ \mathbf{N}_0 & \text{in } [\text{number of electrons } \widehat{\boldsymbol{\lambda}}^3] \ , \\ \boldsymbol{\beta}_0 & \text{in } [\widehat{\boldsymbol{\tau}}^{-1}] \ , \\ \mathbf{F} &= 1 \text{ or } 2 \\ \text{angle } \boldsymbol{\phi} \text{ in radians } , \\ \mathbf{angle } \boldsymbol{\delta} \text{ in radians } , \\ \mathbf{T} & \text{in } [\widehat{\boldsymbol{\tau}}] \ . \end{array}$$

A.2 Coefficients of the Differential Equation

First let us define the following quantities:

$$D_1(h) = D_0 \cdot EXP\left[\frac{h-H_0}{H_1}\right] \quad in \left[\frac{\lambda^2}{\hat{\tau}}\right] ;$$

$$\beta(h) = \beta_0 \cdot EXP\left[\frac{-F(h-H_0)}{H_1}\right] \quad \text{in} \quad \left[\hat{\tau}^{-1}\right] \quad ;$$

$$\cos X = (\sin \phi \cdot \sin \delta) + (\cos \phi \cdot \cos \delta \cdot \cos t') \quad ,$$

where t' is in radians and for the unit of time in Υ (= 24 hours), t' = k · t with $k = 2\pi$ radians/ Υ .

Then, in our special case, the coefficients A, B, E, and Q of the differential equation

$$\frac{\partial N}{\partial t} = A(t,h) \frac{\partial^2 N}{\partial h^2} + B(t,h) \frac{\partial N}{\partial h} + E(t,h,N)N + Q(h,t)$$

are defined by

$$A(h,t) = A(h) = D_1(h) \qquad \text{in } \left[\frac{\lambda^2}{\tau}\right],$$

$$B(h,t) = B(h) = \frac{3D_1(h)}{2H_1} \qquad \text{in } \left[\frac{\lambda}{\lambda}\right],$$

$$D_1(h) \qquad A$$

$$C(h,t) = C(h) = -\beta(h) + \frac{D_1(h)}{2(H_1)^2}$$
 in $[\tau^{-1}]$,

$$D(h,t,N) = 0 ,$$

and so

$$E(h,t,N) = C(h,t) + D(h,t,N) = -\beta(h) + \frac{D_1(h)}{2(H_1)^2}$$

is a function of h only. Q(h,t), the only coefficient dependent both on h t, is of the form

$$Q(h,t) = Q_0 \cdot EXP \left\{ 1 - \frac{h-H_0}{H_1} - (\sec X)EXP[-\frac{h-H_0}{H_1}] \right\} in \left[\frac{\Lambda}{\lambda} - 3/\frac{\Lambda}{\tau} \right] \text{ when } |X| < \pi/2 ;$$

= 0 when
$$|X| \ge \pi/2$$
.

A.3 The Boundary Conditions

The boundary condition $N(h,0)=G_{\underline{i}}$, where $\underline{i}=1$ or 2, at $\underline{t}=0$ and for $0\leq h\leq 1$ is either

$$G_1(h) = N_0 \cdot EXP \left\{ \frac{1}{2} (1 - \frac{h-H_0}{H_1}) - EXP \left[\frac{-2(h-H_0)}{H_1} \right] \right\}$$

or else

$$G_{2}(h) = \begin{cases} 0 & \text{when } 0 \leq h \leq H_{0} \\ \\ N_{0} \cdot \left\{ EXP[-\frac{h-H_{0}}{2H_{1}}] - EXP[-\frac{2(h-H_{0})}{H_{1}}] \right\} & \text{when } H_{0} < h \leq 1 \end{cases}.$$

Both $G_i(h)$ represent the number of electrons/ λ^3 . At the input time one should specify which $G_i(i=1 \text{ or } 2)$ will be used.

For t > 0, the boundary condition at h = 1 is

$$\frac{\partial N}{\partial h} + (\frac{1}{2H_1})N = 0 ,$$

where H_1 is an input parameter already mentioned in the present appendix.

The boundary condition at h = 0 for t > 0 is

$$N(0,t) = 0 .$$

APPENDIX B: USAGE OF THE COMPUTER PROGRAM

B.1 Computer Program

First let us review some basic features of the computer program for the numerical solution of our boundary value problem which should be of interest to its prospective user. Almost all of them have already been mentioned in and are scattered through other parts of this report. However, in order to make APPENDIX B relatively independent from the rest of the report, we summarize this useful information below:

- 1. The program has been coded in the symbolic language (SCATRE) for the IBM 7094 computer of the Digital Computer Laboratory of the University of Illinois.
- 2. Double precision normalized floating point arithmetic is used internally. The mantissa of a double precision floating point number on the IBM 7094 is 54 bits long.
- 3. Three finite-difference methods (backward difference, central difference, and Crank-Nicolson) are incorporated in the program. The user must indicate by an input signal which one of them he intends to use. How to choose values for this signal is explained in the description of the input.
- 4. The central difference method is of experimental nature. Its final acceptance or rejection will depend on the results of further testing and theoretical work. This method uses three time levels and thus has to be started by some two-times-level method which in our use happens to be the backward difference method.

B.2 Composition of the Input Data Deck

By a <u>run</u> we mean an integration (numerical solution) sweep executed from the initial time t=0 through some final value of t, say t_{FN} . Each run may be segmented into one or several <u>stages</u>. One specifies a stage, say the $i\frac{th}{t}$, by fixing a constant time step, Δt_1 , to be used throughout it and by giving its final (or end) time point t_{F1} . In a run consisting of N stages, the t_{F1} must be ordered such that

$$0 < t_{F1} < t_{F2} < \dots < t_{FN}$$
 .

During the execution time the east stage of a run will be recognized by the current value of the so-called <u>exit flag</u>: the value of that flag associated with the last stage should be = 1; for any other stage, it should be = 0.

A machine job will consist of one or several runs depending on for how many runs the input data has been furnished.

Using the terminology introduced above we can now speak of the stage or run data subdecks of a job input data deck. The composition of a typical job input data deck is illustrated by the following diagram.

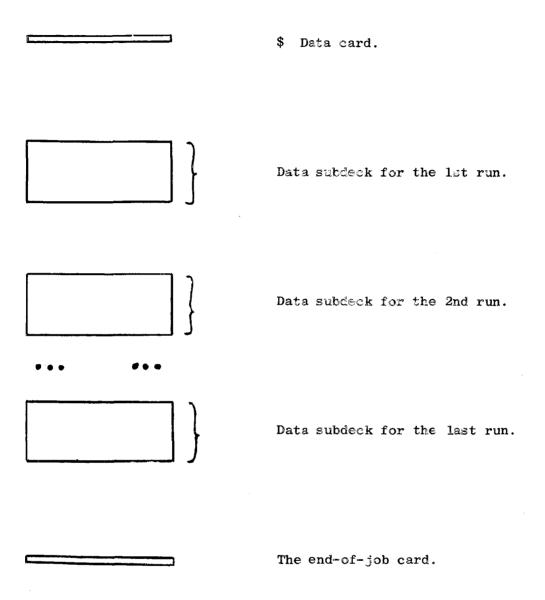


Fig. B.1: Composition of a job input data deck

The "\$ DATA" and the end-of-job cards are always of the same fixed format and should always be present in the data deck.

Warning: the user should become familar with the current rules of the Digital Computer Laboratory concerning other "\$" system cards that may have to be added to or omitted from the job input data deck.

The composition of a run input data subdeck is as follows:

CARD CONTENTS

Run ID (title) card: an arbitrary alpha numeric message in

columns 2-72; "1" should be punched in

col. 1.

Run control card: L; the integration-mode-signal; the

write-mode-signal; BCFLG (= the

boundary condition flag).

 H_0 ; H_1 ; D_0 ; β_0 . Card 1 of floating point numbers:

Card 2 of floating point numbers: Φ; δ; τ.

Card 3 of floating point numbers: $F; N_0; Q_0.$

 t_{Fl} ; $\triangle t_{1}$; $\triangle t_{Wl}$; SWMODE (= the stagewrite-mode signal); EXFLG (= the exit Stage (#1) card:

flag) = 0.

 t_{F2} ; $\triangle t_{2}$; $\triangle t_{W2}$; SWMODE (= the stagewrite-mode signal), EXFLG (= the exit Stage (#2) card:

flag) = 0.

 t_{N} ; $\triangle t_{N}$; $\triangle t_{WN}$; SWMODE (= the stagewrite-mode signal), EXFLG (= the exit Stage (#N) card:

flag) = 1.

Fig. B.2: Composition of a run input data subdeck

The following table provides sufficiently detailed information needed to design and punch the input data cards. In the event that the user is not familiar with the definitions of the I-, E-, and H-fields as used in input format statements, he is advised to consult the SCATRE manual issued by the Digital Computer Laboratory of the University of Illinois.

FIELD		TYPE	SYMBOLIC	
COLUMNS & TYPE	ADJUST	OF INPUT QUANTITY	NAME OF STORAGE LOCATION	INPUT QUANTITY
Ru	ın ID (t	itle) card		
01 (1批)		Alphanumeric	TCARD	Pos. integer "1" should be punched
02-72 (71H)	Arbi- trary	Alphanumeric	TCARD + 6	An arbitrary ID message 71 alphanumeric characters long (including blanks); for example, "THE ELECTRON DENSITY IN THE IONOSPHERE, STUDY NO.XX".
73-80		Blank		
Ru	n contr	ol card (of	fixed point	parameters)
01-06 (16)	Right	Positive integer	L	L = the no. of $\triangle h$ subintervals in $0 \le h \le 1$. Range: $4 \le L \le 256$.
07-12 (16)	Right	Integer	MODE	The flag for determining the mode of the numerical solution. The value 0 >> backward difference method. The value 1 >> central difference method. The value 2 >> Crank-Nicolson method.
13-18	Right	Integer	WMODE	The control flag for writing the input data and the results of the preliminary calculations. The value 0 the input data, h _j -, and H _j -tables written; The value 1 in addition, other preliminary calculations written. Normally, the user should use the value = 0.
19-24 (16)	Right	Integer	BCFLG	The control signal for the choice of boundary conditions at $t = 0$. The value $0 \Rightarrow G_1(h)$; The value $1 \Rightarrow G_2(h)$.
25-80		Blank		

FI	ELD	TYPE	SYMBOLIC	
COLUMNS & TYPE	ADJUST	OF INPUT QUANTITY	NAME OF STORAGE LOCATION	INPUT QUANTITY
Card 1 of floating point numbers				
01-18 (E18.8)	Right	Fl. point	но	H _O in [1,000 km].
19-36 (E18.8)	Right	Fl. point	H1	H ₁ in [1,000 km].
37-54 (E18.8)	Right	Fl. point	DOU	D ₀ in [(1,000 km) ² /hr].
55-72 (E18.8)	Right	Fl. point	BETAOU	β ₀ in [hr ⁻¹].
73-80		Blank		
C	ard 2 of	floating po	int numbers	
01-18 (E18.8)	Right	Fl. point	PHI	φ in [radians].
19-36 (E18.8)	Right	Fl. point	DELTA	δ in [radians].
37-54 (E18.8)	Right	Fl. point	TAUU	τ in [hr].
55-80		Blank		·
C	ard 3 of	floating po	int numbers	
01-18 (E18.8)	Right	Fl. point	F	F = 1.0 or = 2.0 [dimensionless].
19-36 (E18.8)	Right	Fl. point	NO	N_0 in [no. of electrons/(1,000 km ³].
37-54 (E18.8)	Right	Fl. point	QUO	$Q_0 \text{ in } [(1,000 \text{ km})^{-3} \text{ hr}^{-1}].$
55-72 (E18.8)		Blank	:	
Stage card				
01-18 (E18.8)	Right	- Fl. point	TFU	t _F in [hr].
19-36 (E18.8)	Right	Fl. point	DELTU	∆t in [hr].
37-54 (E18.8)	Right	Fl. point	DELTWU	∆t _w in [hr].

FIE COLUMNS & TYPE	LD ADJUST	TYPE OF INPUT QUANTITY	SYMBOLIC NAME OF STORAGE LOCATION	INPUT QUANTITY	
S	tage car	d (continued)		
55-78		Blank			
79 (I1)		Integer		The control signal for writing the output of the stage. The value = 0 or 1 > standard output; The value > 2 > in addition, intermediate quantities dependent on t written; The value > 3 > in addition, the coefficients of the system of linear equations written. Normally, the user should use the value = 0 or 1.	
80 (I1)		Integer	EXFLG	The flag for indicating the last stage of a run. It should be = 1 for the last stage and = 0 for any other stage.	
End-of-job card (to follow the input data subdeck of the last run in a job)					
1 (1H)	,	Alphanumeric	TCARD	"-", the minus sign, should be punched.	
02-11 (10H)		Alphanumeric	TCARD + 6	The message "END OF JOB" should be punched.	
12-80		Blank			

APPENDIX C: FLOWCHARTS

The flow charts contained in this appendix are presented in the same order as the corresponding subprograms appear in the program. The name by which a subprogram, including the master control, is referred to is its symbolic entry address. For the convenience of the user, we list next the names of all subprograms in the order indicated above:

```
MCNTRL (the master control)
ERREX
IA000
IB000
SB000
EQ000, EQ100
ME000, ME100, ME200, ME300, ME400, ME500, ME600
PR000, PR100
DE000
WC000
WT000, WT100, WT200
WP000
WX000
```

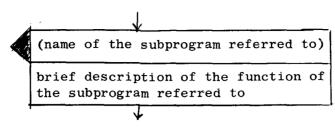
Each subprogram is entered from a higher level subprogram (the master control in this respect is the highest level subprogram) by using a basic linkage of the following type:

```
a TSX (name of subprogram), 4
```

a + 1 (normal exit)

There are subprograms which do not return the control to the location $\alpha+1$. Such cases are clearly indicated.

A reference to a lower level subprogram from a higher level subprogram is indicated by



in the flowcharts contained in this appendix.